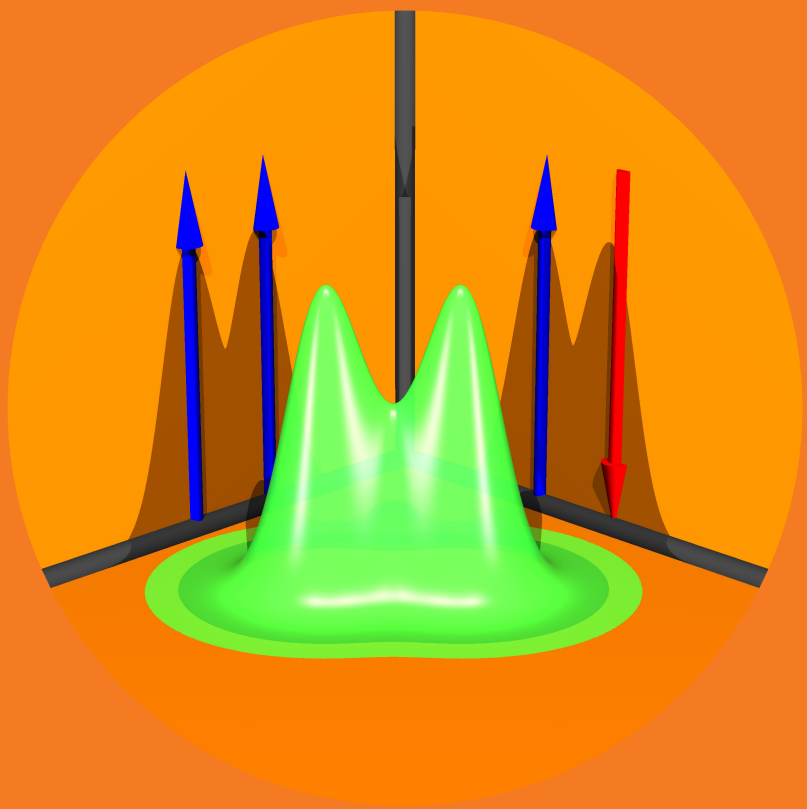
Department of Applied Physics

Dynamics and decoherence in two-electron quantum dots

Jani Särkkä



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Jani Särkkä

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Aalto University
School of Science
Department of Applied Physics
Quantum Many-Body Physics Group

Supervisor
Professor Risto Nieminen

Instructor
Adjunct Professor Ari Harju

Preliminary examiners
Adjunct Professor Esa Räsänen, University of Jyväskylä, Finland
Professor Kalle-Antti Suominen, University of Turku, FInland

Opponent
Professor Jason Petta, University of Princeton, USA

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Jani.Sarkka@tkk.fi

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Abstract

Aalto University, P.O. Box 11000, FI-00076 Aalto www.aalto.fi

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Semiconductor quantum dots have been studied experimentally and theoretically for two decades. With the help of modern experimental techniques, it is possible to control the number of electrons in the dots at single-electron level, and one can apply different confinement potentials and vary the strength of the external magnetic field. These properties make quantum dots ideal for studies of quantum mechanical effects. The spin of the confined electron is a natural candidate for a quantum bit, as the z-component of spin can have two different values, up or down, making quantum dots suitable to be used as a building block of the quantum computer. The decoherence of the quantum states is a factor that has to be taken into account, and for this reason it is important to study the time-dependent phenomena in quantum dots.

This Thesis studies the dynamics of two electrons confined in two dimensions in a double quantum dot or in a quantum ring. We study the decoherence of the two-electron states by calculating the dynamics of the two-electron system and compare the results with experimental data. We apply exact diagonalization methods for the numerical evolution of the dynamics. The Coulomb interaction of the two confined electrons is taken into account. For large electron numbers, the calculation of the dynamics with full exact diagonalization becomes too heavy, but for two electrons, the dynamics can still be calculated exactly with reasonable computing resources.

This Thesis explains some decoherence measurements with numerical results. We study especially the hyperfine interaction of the nuclear spins of the surrounding material with the spins of the confined electrons and the effects of nuclear spin polarization. We propose novel control schemes that can be used to manipulate the two-electron states in quantum dots. Our results may prove to be useful for experimentalists in the development of quantum dot systems towards a realization of a semiconductor-based quantum computer.

Keywords quantum dots, quantum computation

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Tiivistelmä

Tekijä
Jani Särkkä

Väitöskirjan nimi
Kaksielektronikvanttipisteiden dynamiikka ja dekoherenssi

Julkaisija Perustieteiden korkeakoulu

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Tiivistelmä

Puolijohdekvanttipisteitä on tutkittu kokeellisesti ja teoreettisesti viimeisten kahden vuosikymmenen aikana. Modernit kokeelliset menetelmät mahdollistavat kvanttipisteen elektronien lukumäärän kontrollin yksittäisten elektronien tarkkuudella. Kvanttipisteen potentiaalia ja ulkoisen magneettikentän voimakkuutta voidaan säätää sopivaksi. Nämä ominaisuudet tekevät kvanttipisteistä sopivia kvanttimekaanisten ilmiöiden tutkimiseen. Kvanttipisteeseen sidotun elektronin spini on luonnostaan sopiva kvanttibitiksi, sillä spinin z-komponentti on kvantittunut kahteen arvoon, ylös tai alas. Kvanttipisteitä voidaan siten käyttää kvanttitietokoneen rakennusosasina. Kvanttitilojen dekoherenssilla on suuri merkitys, joten aikariippuvat ilmiöt kvanttipisteissä ovat tärkeä tutkimuskohde.

Väitöskirjassa käsitellään kahden elektronin dynamiikkaa kaksoiskvanttipisteessä ja kvanttirenkaassa. Tutkimme kaksielektronitilojen dekoherenssia laskemalla kaksielektronisysteemin dynamiikan ja vertaamme tuloksia kokeellisiin mittauksiin. Sovellamme eksaktin diagonalisaation menetelmää dynamiikan numeeriseen laskentaan ottaen huomioon kahden elektronin Coulombin vuorovaikutuksen. Suurille elektroniluvuille dynamiikan laskenta on liian raskasta eksaktia diagonalisaatiota käyttäen, mutta kahden elektronin dynamiikka on vielä laskettavissa eksaktisti kohtuullisilla laskentaresursseilla.

Väitöskirja selittää joitakin dekoherenssimittauksia numeeristen laskujen avulla. Tutkimme varsinkin ympäröivän aineen ydinspinien ja kvanttipisteeseen sidottujen elektronien spinien vuorovaikutusta ja sen vaikutusta spinien polarisaatioon. Esitämme uusia kontrollimenetelmiä kvanttipisteiden kaksielektronitilojen käsittelyyn. Tulokset hyödyttävät kokeellisia tutkijoita, jotka kehittävät kvanttipisteitä puolijohdepohjaisen kvanttitietokoneen rakentamista varten.

Avainsanat kvanttipisteet, kvanttilaskenta

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Preface

The research for Thesis has been carried out during the years 2006-2010 in the Department of Applied Physics at the Aalto University School of Science, formerly known as Laboratory of Physics at the Helsinki University of Technology. The author has been a member of the Quantum Many-Body Physics (QMP) group, which is a part of the Center of Excellence in Computational Nanoscience (COMP) funded by the Academy of Finland. QMP group has also been affiliated to Helsinki Institute of Physics since 2008.

I am grateful to my supervisor, Aalto Distinguished Professor Risto Nieminen, for giving me the opportunity to perform graduate studies in COMP and providing excellent working conditions. I am deeply indebted to my instructor Adjunct Professor Ari Harju for presenting interesting research problems and helping in computational problems and in manuscript preparation. He has created a relaxed and informal atmosphere in the QMP group and was always available, when help was needed. The pleasant working environment has been enriched by the people I have shared my office with: Markku Stenberg, Eero Tölö, Christian Webb, and Jaakko Nissinen. Special thanks to Mikko Ervasti for commenting the manuscript of the Thesis. The interesting discussions during the lunch with members of QMP group have formed a refreshing break during the workdays.

The financial support in the form of scholarships from Magnus Ehrnrooth foundation, Finnish Cultural Foundation and Research Council of Helsinki University of Technology is gratefully acknowledged.

Finally, I want to thank my family for the support and encouragement during my graduate studies.

Espoo, April 2011

Jani Särkkä

Contents

List of publications

This Thesis consists of an overview and the following publications:

I J. Särkkä and A. Harju,
Spin dynamics in a double quantum dot: Exact diagonalization study,
Physical Review B **77**, 245315:1-6 (2008).

II J. Särkkä and A. Harju,
Effect of nuclear polarization on spin dynamics in a double quantum dot,
Physical Review B **79**, 085313:1-5 (2009).

III J. Särkkä and A. Harju,
Control of a two-electron double quantum dot with an external magnetic field,
Physical Review B **80**, 045323:1-5 (2009).

IV J. Särkkä and A. Harju,
Control of a two-electron quantum ring with an external magnetic field,
Physica E **42**, 844-847 (2010).

V J. Särkkä and A. Harju,
Charge dynamics in two-electron quantum dots,
Journal of Physics: Conference Series **245**, 012019:1-4 (2010).

VI J. Särkkä and A. Harju,
Spin dynamics at the singlet-triplet crossings in double quantum dot,
New Journal of Physics **13**, 043010:1-10 (2011).

The research presented in this Thesis has been carried out at the Helsinki University of Technology in the Laboratory of Physics during the years 2006-2007 and in the Department of Applied Physics during the years 2008-2010.

The author has had an active role in all the research reported in this Thesis. He has been one of the major contributors to the development of the computer programs employed to calculate the results presented in all publications. The author has designed the work and performed the calculations reported in all publications, and has had the main responsibility for writing the publications.

Chapter 1

Introduction

The rapid progress of the semiconductor technology during previous decades has enabled a staggering development of computers, multiplying their computing capacity. Our society is nowadays fully dependent on information technology, and the effects of this development on our daily life, both work and free time, have even surpassed the visions of the past science enthusiasts.

As the size of the semiconductor chips has constantly diminished in order to reach higher computing efficiency, the quantum mechanical effects must be taken into account. In the design of small-scale devices, the quantum effects do not have to be seen only as a nuisance. One can harness the complexity of the quantum world to increase parallelism in computation, and solve problems that today are computationally impossible to be solved. This new kind of computer, quantum computer, is now an object of wide theoretical and experimental interest.

Semiconductor quantum dots have emerged as one of the most popular candidates for a quantum bit, a building block of the quantum computer. The number of electrons confined in the quantum dot can be controlled with one-electron accuracy. The form of the confinement potential can be controlled with external

voltage. The spins of the confined electrons are ideal states for quantum computing, as the spin is quantized to two opposite directions, forming a natural quantum bit.

The dynamical behavior of these few-electron quantum dots has been experimentally studied during recent years, as the measurement techniques have developed to a reasonably high level. Theoretically, even the calculation of the dynamics of two interacting electrons is a heavy task in an exact fashion. In computational physics, the interaction of the electrons is often approximated by using, e.g., Hartree-Fock or density-functional methods.

In this Thesis, the time-dependent properties of two-electron quantum dots have been calculated using the so-called exact diagonalization method. This method solves the Schrödinger equation with great accuracy, limited only by the size of the numerical basis. The dynamics of the states of the confined electrons are calculated and compared with experimental results on similar systems.

This Thesis is organized as follows. Chapter 2 discusses general concepts of quantum computation. Chapter 3 includes a presentation of the physical foundations of electron spin, quantum dots, and the physical phenomena, especially interaction with environmental degrees of freedom that are relevant to semiconductor quantum dots. The implementation of electron spin qubits is also discussed. Chapter 4 deals with the details of the computational methods that are used in the calculation of the dynamics of the electron states. Chapter 5 summarizes the content of the Thesis.

Chapter 2

Quantum computation

The development of modern computers has initiated an enormous change in our society. Sophisticated techniques have enabled an ever increasing number of transistors in an integrated circuit, fulfilling the prediction of Moore's law. Despite this success of information technology, the complexity of many mathematical and physical problems exceeds the capability of classical computers. One possible way to solve these challenging problems is to design and realize a computer that utilizes quantum mechanical properties to enhance the capacity of the information processing. Feynman published in 1982 a paper [1] that proposed the use of quantum systems in computing. His idea was developed further by Deutsch [2]. A very important incentive to the development of quantum computation was the algorithm presented by Shor for the factorization of large integers to prime numbers [3]. This method scales much better than the present classical methods with the size of the integers, so that factorization of very large integers becomes possible with quantum computers. Many encrypting methods used in modern communication are based on the difficulty of finding the prime factors of large integers. Shor's algorithm opened the pockets of investors who were interested in the possibility of breaking the encryption methods. From a physicist's point of view, the simulation of quantum systems with a quantum

computer [1] would mean a huge step forward in the computational quantum physics.

The bit in a classical computer is either 0 or 1. In a quantum computer, the classical bit is replaced with a quantum bit (qubit) that is in an arbitrary superposition of two states 0 and 1 such that $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where the two complex numbers squared sum up to one $|\alpha|^2$+$|\beta|^2 = 1$ for proper normalization. When the state of the qubit is measured, it collapses to state $|0\rangle$ with probability $|\alpha|^2$ and to state $|1\rangle$ with probability $|\beta|^2$. Another difference between classical and quantum computers is the entanglement of composite quantum systems. For example, the two-particle state $(|01\rangle + |10\rangle)/\sqrt{2})$ cannot be described as a tensor product of two states, i.e., the states are not separable. If the state of one particle is measured, the unmeasured one also collapses to $|0\rangle$ or $|1\rangle$, even if the particles are spatially far away. The decoherence of the qubit with environment destroys the qubit-qubit entanglement. The preservation of entanglement properties in quantum computers thus necessitates control of decoherence.

The power of quantum computing lies in quantum parallelism. If a system of several qubits is initially in a superposition of many states and an operation is made, the system is in the superposition of all possible final states. The quantum computer has performed the calculation for all initial values simultaneously. The number of superposition states increases exponentially with the number of qubits. Hence, for larger number of qubits,the quantum computer beats a classical computer in computing power. Still, this parallelism might seem useless, because when the qubit state is measured, it collapses to one state and information on the other states is lost. That makes careful design of quantum algorithms very important. The quantum parallelism can be efficiently used for some problems, as prime factorization, but for other problems classical computer still remains the best tool.

The requirements that have to be fulfilled for the physical implementation of

a quantum computer are summarized in the five criteria defined by David DiVincenzo [4]. The first criterion states that for the realization we should have *a scalable physical system with well characterized qubits*. The easiest way to do this is to use a two-level system with only two states. An example would be a single photon, which has two polarization states (horizontal and vertical) [5]. The two states form the basis vectors of the qubit, $|0\rangle$ and $|1\rangle$. The number of qubits should be large, and it should be possible to manipulate each qubit independently of the other qubits and also perform two-qubit operations for the creation of entangled qubit states.

Several different realizations based on two-level systems have been the focus of experimental qubit studies. Some other examples of qubit states, besides the photon, are single-electron spins, electron charge in a quantum dot (0 or 1) [6], nuclear spins [7, 8], Josephson charge qubits (0 or 1 Cooper pairs) and Josephson flux qubits (clockwise or counterclockwise direction of supercurrent) [9]. Josephson charge qubit was the first physically realized qubit [10]. The scalability of these systems is often straightforward, but in practice many problems have to be solved before large numbers of working qubits are achieved.

The second criterion demands *the ability to initialize the state of the qubits to a simple initial (fiducial) state such as* $|00...0\rangle$. For many realizations, the qubits are in the ground state when the temperature is low. For electron spins, one can utilize a high magnetic field and wait until the spin system has relaxed to the ground state.The quantum state should be preserved so long that quantum computation can be made. This is the reason for the third criterion that requires *long relevant decoherence times, much longer than the gate operation time*. The qubit interacts with its environment and causes the decay of the off-diagonal elements of the density matrix. When the number of qubits increases, the decoherence is quite likely enhanced. For efficient qubit operations, the gate operation time should be many orders of magnitude shorter than the decoherence time. The aim of experimentalists is to prolong the decoherence times and shorten the gate

operation times to achieve working quantum computation.

Running different quantum computing algorithms in a quantum computer requires suitable gate operations. In order to construct these operations, the fourth criterion must be fulfilled, the system should have *a "universal" set of quantum gates*. At a first glance, it seems that the performance of a complicated multi-qubit operation would not always be possible, but the theorem of Barenco *et al.* [11] states that any multi-qubit operation can be reduced to single-qubit operations and CNOT gates. In the CNOT (controlled NOT) operation, the second qubit is flipped if and only if the first qubit is 1. It is thus sufficient to design single-qubit gate operations and a CNOT two-qubit gate for a realization. The decomposition of complex multi-qubit gates to single-qubit gates is an important branch of quantum computing research. There are various different ways to decompose quantum operations. For different realizations, the experimentally possible operations restrict the used decomposition. For electron spins, single-spin rotations with oscillating magnetic field and exchange control of two-spin qubit is one working operation method [12, 13].

The fifth criterion states that we have to find out the result of the calculation the quantum computer has made. That means that the system should have *a qubit-specific measurement capability*. In practice, it is not possible to achieve 100 % efficiency in the measurement, since the decoherence with the environment, accuracy of the measurement method and other factors limit the visibility of the final state. The qubit state can be preserved if the state of another system, correlated with the qubit, is measured. This is called non-invasive measurement. Often reliable results are obtained by repeating the measurement. This is the case for instance in a measurement, in which we have to find the coefficients α and β of a qubit superposition state. The electron spin is often measured with charge-sensing techniques, where the charge distribution depends on the spin state. This method is called spin to charge conversion.

Chapter 3

Spins in quantum dots

3.1 Electron spin

In the beginning of the previous century, the measurement of atomic spectra emerged as a test of quantum mechanical theories. The Schrödinger equation [14] explained the spectrum of the hydrogen atom. It turned out that three quantum numbers were needed to explain the electron states: shell number n, orbital number l and orbital angular momentum number m. The spectrum of the electromagnetic radiation absorbed and emitted by an atom originates from the transitions between certain pairs of electron states with different quantum numbers, restricted by the transition rules.

In the presence of an external magnetic field a problem emerged: the spectrum could not be explained with the three quantum numbers. The spectral lines measured without magnetic field were split into more lines. This effect is called the fine structure splitting. Only when a fourth quantum number was introduced by Wolfgang Pauli to the theory, these new splittings could be understood. This new quantum degree of freedom - spin - is the basis for Pauli exclusion principle [15]. Two electrons cannot occupy the same quantum state, hence their spins should

be different if the three other quantum numbers are the same. George Uhlenbeck and Samuel Goudsmit together [16] and Ralph Kronig independently proposed in 1925 (although Kronig did not publish his work, discouraged by Pauli) that the electron spin originates from its self-rotation, creating an angular momentum vector for the electron. Depending on the direction of the rotation, the spin is either $\hbar/2$ or $-\hbar/2$.

If one assumes that the electron is a charged sphere, the radius of the electron can be approximated by setting the relativistic rest energy of the electron $m_e c^2$ equal to the potential energy of a sphere with total charge e and radius r_e, which is proportional to $\frac{1}{4\pi\epsilon_0}\frac{e^2}{r_e}$. Solving this equation, we obtain the classical electron (Lorentz) radius $r_e = 2.8$ fm. If the electron magnetic momentum is interpreted to be caused by the rotation of a charged sphere with Lorentz radius, the velocity of the surface of the sphere would be about 800 times the speed of light. Clearly, this is not a valid interpretation for spin. Instead, the electron spin is a relativistic quantum-mechanical effect that is not related to any rotation, and the electron can be thought as a point particle. Also the spins of proton and neutron are quantum mechanical effects and not related to any actual rotation of particles. Pauli formulated his spin theory quantum-mechanically in 1927 and introduced Pauli spin matrices [17]. Finally, Paul Dirac presented the relativistic equation for the electron in 1928 [18]. The electron spin emerges naturally in the solution of the Dirac equation as a fourth quantum number of the point-like electron.

The first experimental demonstration of the existence of the electron spin was made in 1922 by Otto Stern and Walter Gerlach [19,20]. In their experiment (see Fig. 3.1), a beam of silver atoms was led through an inhomogeneous magnetic field. The magnetic field splits the beam into two parts. The beams hit a plate, where an observable pattern is formed. If the spins of the silver atoms were distributed randomly, the beam would be spread continuously. But the spins have only two opposite values, and the beam is split into two parts, leaving a gap between the spin-up and spin-down beams. Actually, at the time of the Stern-

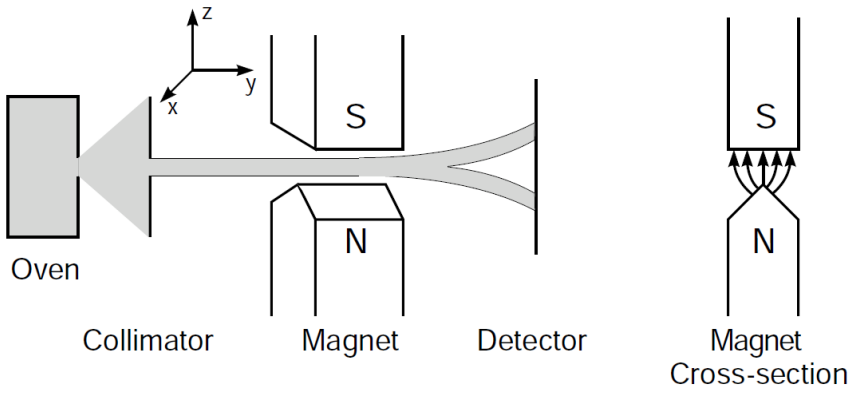

Figure 3.1: The setup of Stern-Gerlach experiment. The magnet cross section shows the inhomogeneous magnetic field used in the experiment.

Gerlach measurement, the existing model of the silver atom supposed that the total angular momentum of the silver atom comes from its only valence electron that has nonzero orbital angular momentum. Stern and Gerlach interpreted that they measured the spin of the silver atom and thus confirmed the quantization of angular momentum proposed by Niels Bohr and Arnold Sommerfeld [21]. Only later it was found out that in the silver atom, the orbital angular momentum of the valence electron is zero, and the Stern-Gerlach experiment is explained by the spin of the valence electron.

3.2 Quantum dots

The term quantum dot was first used in a publication of Reed in 1988 [22] in the context of semiconductor nanostructures. The name originates from the confinement of a small number of electrons in a tiny volume, “dot”. Nowadays, quantum dots can be divided into two categories. Chemists have made colloidal

quantum dots, which are produced in large quantities using chemical reactions. They are passivated by organic molecules on their surface. The compound used is often cadmium selenide or cadmium telluride. They have been used in bio-imaging applications and in light-emitting diodes. As cadmium is a toxic material, other options for quantum dot materials are actively searched.

The other group of quantum dots, relevant to this Thesis, consists of epitaxial quantum dots, defined by electrostatic gates on substrates. Alternatively, they can be fabricated by self-assembling methods. Even a molecule or a nanoparticle can be trapped between electrodes so that a quantum dot is formed.

The essential properties of quantum dots are that the energy levels of charge carriers are quantized and the separation of energy levels increases when the size of the dot decreases. When the electrons are confined in two dimensions, the screening of the Coulomb interaction becomes less effective. Hence, the electron-electron interaction becomes prominent and Coulomb blockade of the electrons is observed.

The quantum dots are also called artificial atoms, because of their discrete energy levels. Quantum dots have similar shell structure and optical selection rules to real atoms. Coupled quantum dots are also sometimes called artificial molecules.

Studying the properties of interacting electron gas is very demanding due to electron-electron interaction and interaction between electron and the environment. If the dimensions of the electron system are reduced, the experimental difficulties are more easily overcome. If the movement of the electron gas is restricted in one dimension, it is called two-dimensional electron gas (2DEG). The energy levels for motion in the direction of the confinement are then quantized. If the confinement is sufficiently strong, the energy levels are so widely separated that the motion in the confinement direction need not to be taken into account. The first realization of 2DEG was electrons floating on the surface

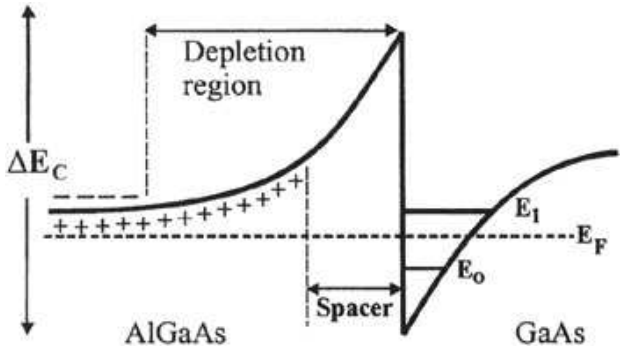

Figure 3.2: A sketch of the conduction band structure of a GaAs/AlGaAs heterojunction showing the confined states at the interfaces, the Fermi energy, the spacer, the depletion region, and the conduction band offset (adapted from Ref. [24] by Manasreh).

of liquid helium [23]. Nowadays electrons moving on a graphene sheet are intensely studied, as the mobility of the electrons in graphene is exceptionally high.

The realizations of 2DEG relevant to this Thesis have been made using semiconductor heterostructures. The structure consists of AlGaAs and GaAs, grown by molecular-beam epitaxy. AlGaAs is an alloy of AlAs and GaAs having the chemical formula $Al_xGa_{1-x}As$. It is n-doped with Si, causing an excess of electrons. When AlGaAs and GaAs are connected, the energy bands change so that a triangular quantum well forms at the interface (Fig. (3.2)). The excess electrons are confined in this well. A region in AlGaAs close to the interface, spacer, is left undoped so that the donors do not scatter electrons of the 2DEG. This method is called modulation doping.

In order to make a quantum dot in a 2DEG, we have to create a quantum well where the electrons are further confined in the directions of the 2DEG. This can be done either by etching a vertical pillar out of the heterostructure (vertical quantum dot) of by using gate electrodes on the surface of the heterostructure

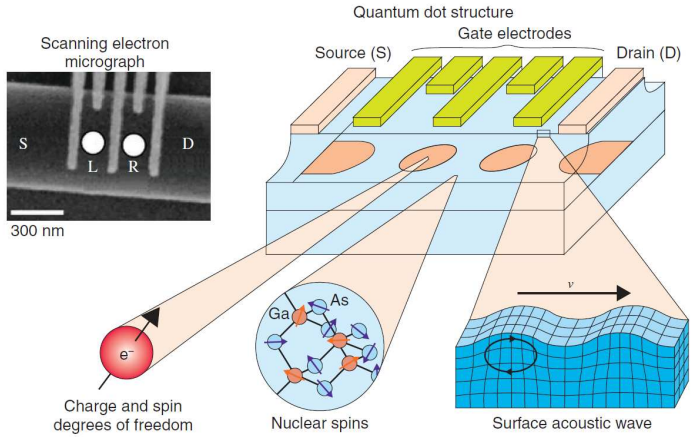

Figure 3.3: Double quantum dot device (adapted from Ref. [25] by Fujisawa). Electrons in the dots interact with nuclear spins of GaAs, and with the lattice phonons and surface acoustic waves.

(lateral quantum dot). In Figure 3.3, the layout of a lateral double quantum dot is presented in a general level. The fabrication of quantum dots is often done by the electron-beam lithography. The electrostatic gates are designed so that during the depletion of the 2DEG, electrons can be confined in small islands, forming quantum dots. These dots are connected to the electron gas reservoirs with low-resistance contacts. The electronic properties of the dot can be measured by attaching current and voltage probes to the reservoirs. The dot is also coupled capacitively to gate electrodes that are used to tune the electrostatic potential of the dot with respect to the reservoirs. The observation of quantum phenomena in these setups demands low temperatures, such that the operating temperatures should be below 1 K. In practice, the temperatures of the experiments are below 100 mK.

The control of the number of confined electrons in the quantum dot reached a high level, when the electron number was reduced to few electrons, even to one or zero, by Ashoori *et al*. in 1992 [26]. They were able to measure the mag-

netic field dependency of the few electron ground states for different electron numbers [27]. In 2000, Ciorga *et al.* [28] published their results of a lateral single quantum dot. They measured the electron number in the dots by analyzing the current that was transported through the dot. In 2003, Elzerman *et al.* [29] showed that they could control electron number in a double quantum dot. They measured the charge with two quantum point contacts (QPC) close to the dots. The conductance of QPCs is very sensitive to the charge in the dots. The benefit of this method is that the charge measurement does not affect the charge states of the dots, and this measurement technique has since become the most popular one.

The confinement potential of the dot can also be created with surface acoustic waves (SAW), which propagate on the surface of an elastic material. The amplitude of the waves decays as a function of the distance from the surface. The difference to the gate-defined electrostatic dots is that the SAW potential minima move. This would enable information transfer of the dot states at the speed of SAWs. A single-electron SAW quantum dot has already been realized [30–33], but multielectron SAW dots remain to be seen.

3.3 Two-electron double quantum dots

The development of electrostatic dots has enabled the control of the confinement potential and number of electrons in the dots to a high degree. For two-electron states in the dots, the Pauli exclusion principle plays a significant role, as the state of two electrons with parallel spins in a single dot has much higher energy than the state where the electrons with parallel spins are in different dot minima. The measurement methods allow to detect the spin states of the electrons. Hence, the study of spin states and Landau-Zener transitions between them forms an important part of this Thesis.

3.3.1 Spin states in two-electron double quantum dots

We set the number of confined electrons in the quantum dot to two and choose a potential that has two minima that are so deep that electrons are confined in these minima. This kind of double-minimum quantum dot is called a double quantum dot. Then the electrons have two possible configurations, one electron in each dot or both electrons in the same dot. The Hamiltonian of two interacting electrons confined in two dimensions is

$$H = \sum_{i=1}^{2} \left[\frac{(\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i))^2}{2m^*} + V_{\text{ext}}(\mathbf{r}_i) + g^*\mu_B \mathbf{B} \cdot \mathbf{S}_i/\hbar \right] + \frac{e^2}{\epsilon r_{12}}, \tag{3.3.1}$$

where $\mathbf{r}_i$ are the coordinates of the electrons, $\mathbf{A}$ is the vector potential of the external magnetic field perpendicular to the plane of the electrons, $\mathbf{S} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$ is the spin operator with the Pauli spin matrices σ_i, and $\mu_B = \frac{e\hbar}{2m_e}$ is the Bohr magneton. The values of the material parameters in GaAs are the effective electron mass $m^* = 0.067m_e$, the effective electron gyromagnetic ratio (Landé factor) $g^* = -0.44$, and the dielectric permittivity $\epsilon = 12.7\epsilon_0$. The external potential V_{ext} confines the electrons. Experiments in vertical dots have indicated that a parabolic confinement potential is a good approximation for the dot potential [34].

The state space of two spin 1/2 particles is spanned by four states that include all possible spin orientations: both spins up $|\uparrow\uparrow\rangle$, both spins down $|\downarrow\downarrow\rangle$, first electron spin up and second electron spin down $|\uparrow\downarrow\rangle$, and vice versa $|\downarrow\uparrow\rangle$. The spin eigenstates of S^2 and S_z of this two-spin system are the antisymmetric singlet state $|S\rangle$ and three symmetric triplet states $|T_-\rangle$,$|T_0\rangle$ and $|T_+\rangle$ [20], which

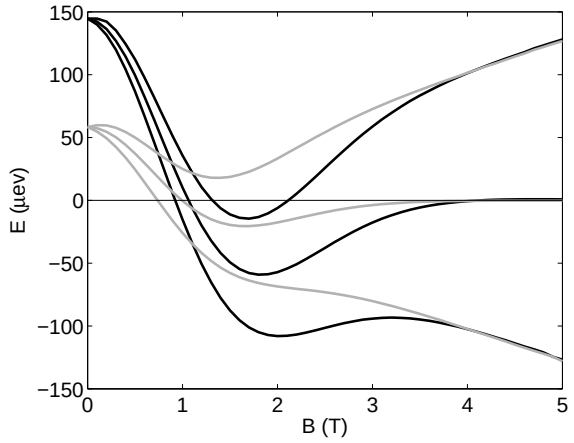

Figure 3.4: Energies of triplet states T_-, T_0 and T_+ as a function of the external magnetic field. The distance of the dots is 40 nm (black) and 50 nm (grey).

are defined as

$$\begin{aligned} |S\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\ |T_+\rangle &= |\uparrow\uparrow\rangle \\ |T_0\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |T_-\rangle &= |\downarrow\downarrow\rangle\,. \end{aligned}$$

As the Hamiltonian of Eq. (3.3.1) commutes with S^2 and S_z, the singlet and triplet states are eigenstates of this Hamiltonian. The total spin for singlet state is $S = 0$ and for triplet state $S = 1$ in units of $\hbar$. In the presence of external magnetic field, the triplet states are separated by the Zeeman energy $g^*\mu_B B$. In a zero magnetic field, the singlet state is the ground state. The dependence of the triplet-singlet energy difference $E_T - E_S$ on the magnetic field is shown in Fig. 3.4.

The energy difference between the S and T_0 states is called the exchange en-

ergy J. In the symmetric triplet states, the electrons are more separated from each other than in the singlet state, because the orbital part of the triplet wave function is antisymmetric. The Coulomb repulsion energy of the electrons becomes smaller and the exchange energy increases. The exchange energy depends strongly on detuning voltage. The singlet and triplet states can be made to cross, so that the triplet becomes the ground state, with a suitable detuning. The states S and T_0, although both have opposite spins in different dots, can be identified through their different charge distribution, which is observed by the charge sensing quantum point contact. Another method to observe the spin state is to use the Pauli spin blockade.

The Pauli exclusion principle prevents electrons with parallel spins occupying the same dot. When a current is led through the quantum dot, the current depends on the spin of the passing electron due to the Pauli exclusion. The effect depends on the direction of the current. If the electron passes the double dot coming from the right hand side of the dot in the sequence with occupations (0,1)→(0,2)→(1,1)→(0,1), the first transition is possible only in the case of opposite spins. If the electron comes from the left hand side, the current has the opposite direction and the sequence is (0,1)→(1,1)→(0,2)→(0,1). Now if, after the first transition, the electrons are in a singlet state, the electron in the left dot is able to make a transition to the right dot. If the electrons are in the triplet state, the triplet state of the two electrons in the same dot has so high energy that the transition is not possible. The singlet and triplet states can be measured using this method. In practice, applying current to the system enhances the coupling of the quantum dot with the environment. In the measurements that are analyzed in this Thesis, the observation of the singlet and triplet states is made with quantum point contacts, as this is a less invasive method.

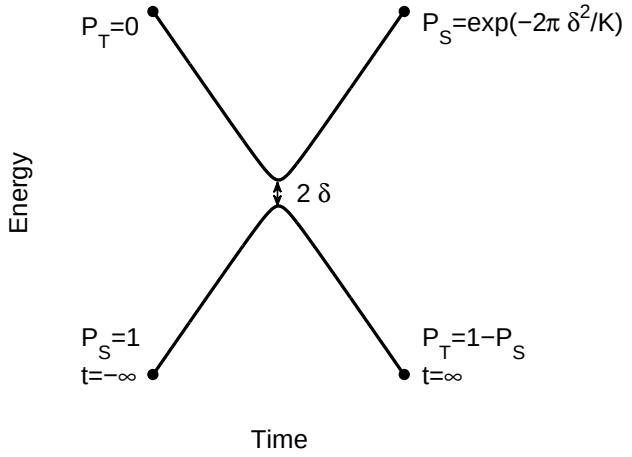

Figure 3.5: Landau-Zener transition. The coupling strength of the two states is δ and the time derivative of the energy difference between the states is K.

3.3.2 Landau-Zener transition

The singlet-triplet transitions, depicted in Fig. 3.4, can be considered as nonadiabatic transitions in a two-level system. Although the singlet and three triplets constitute four levels in total, in the vicinity of the singlet-triplet crossing points the system can be treated as a two-level system and the singlet-triplet transitions can be studied using the Landau-Zener formula for transition probability.

Nonadiabatic transitions between energy levels were actively studied in the 1930s. Four scientists (Lev Landau [35], Clarence Zener [36], Ernst Stückelberg [37] and Ettore Majorana [38]) found in 1932 independently of each other a formula that gives the probability for a transition in the crossing of two energy levels. The formula has been named after the first two scientists as the Landau-Zener formula.

We model the Landau-Zener transition with an effective two-level system where

the energies of the states depend linearly on time and cross each other. The states have a coupling of strength δ. This coupling causes a splitting of 2δ at the crossing of energy levels (see Fig. 3.5). The dynamics of this two-level system can be described with a 2×2 Hamiltonian matrix

$$H = \begin{pmatrix} 0 & \delta \\ \delta & \Delta E \end{pmatrix}, \tag{3.3.2}$$

where ΔE is the energy difference of the two levels. The state is given in the two-level basis as $\psi = (\alpha_1 \ \alpha_2)^T$. Inserting this state into the Schrödinger equation (we set $\hbar$=1) $i\frac{\partial \psi}{\partial t}$=$H\psi$, and taking into account the linear time dependence of the energy difference $\Delta E = Kt$, we obtain a differential equation for α_1,

$$\frac{\partial^2 \alpha_1}{\partial t^2} + iKt\frac{\partial \alpha_1}{\partial t} + \delta^2 \alpha_1 = 0. \tag{3.3.3}$$

We initialize the system so that only one state is occupied, $|\alpha_1(t = -\infty)|^2 = 1$. The transition probability is obtained from the probability of the initial state at $t = \infty$. The asymptotic value can be derived using different approaches (e.g., see Ref. [39]), giving the famous Landau-Zener formula

$$P_S = |\alpha_1(t = \infty)|^2 = \exp\Big(-\frac{2\pi\delta^2}{|K|}\Big), \tag{3.3.4}$$

where the transition probability depends only on the coupling δ and on the speed of the energy change K. If the system is in the initial state in the beginning and the speed is slow, the transition is adiabatic and the system remains in the corresponding ground state. If the speed is high, the system does not have time to make the transition and the other state remains unoccupied. For speeds in the intermediate range, the system is in the end a superposition of two states.

3.4 Interaction between spin and environment

The electron spin is only weakly coupled to the external magnetic field. Also, the coupling of the electron spin to the electric field is only indirect. An exception is the two-electron quantum dot, where the splitting of the singlet and triplet states depends strongly on the external voltage. In semiconductor quantum dots, the most important interactions affecting the spins of the confined electrons are the spin-orbit interaction and the hyperfine interaction with the nuclear spins of the surrounding atoms in the semiconductor.

3.4.1 Spin-orbit interaction

When an electron with momentum $\mathbf{p}$ moves in an electric field $\mathbf{E}$ (due to external field or charge distribution in the semiconductor), the spin of the electron is affected by a magnetic field that arises in the direction of $\mathbf{E} \times \mathbf{p}$. In crystal structures with bulk inversion asymmetry, the effects of electric fields originating from the charges sum up to a so-called Dresselhaus term [40]. If there are asymmetric confining potentials in the materials, they cause structural inversion asymmetry. This is the case in the two-dimensional electron gas at the GaAs/AlGaAs heterointerface. This asymmetry gives rise to another contribution to the spin-orbit interaction called the Rashba term [41]. Spin-orbit interaction changes the Landé factor from its normal value $g^* = 2$. In GaAs, the Landé factor even changes its sign, having the value $g^* = -0.44$ [42].

In quantum dots, one would expect that the spin-orbit interaction does not play a role, as the size of the quantum dot is smaller than the spin-orbit scattering length. However, it turns out that the spin-orbit coupling couples states that have different orbital and spin parts. In two-electron double quantum dots, singlet and triplet states are coupled due to this reason (albeit S and T_0 states are coupled only in higher order). The spin-orbit interaction is in many cases the dominant

spin-environment interaction, because the hyperfine interaction is not present in semiconductor materials with zero nuclear spin.

3.4.2 Hyperfine interaction

Inside an atom, the spins of the electrons interact mainly with the spin of the nucleus of the same atom. In a quantum dot, the spin of a confined electron interacts with many nuclear spins in the host material, because the wave function of the confined electron overlaps with several surrounding atoms. For example, in GaAs quantum dots, the electron spin interacts with 10^6 nuclear spins [43].

The interaction mechanism between electron and nuclear spins is the Fermi contact hyperfine interaction

$$H_{hf} = \sum_{k}^{N} A_k \mathbf{I}_k \cdot \mathbf{S}, \tag{3.4.1}$$

where $\mathbf{I}_k$ and $\mathbf{S}$ are the spin operators for nucleus k and the electron spin, respectively [44]. The coupling of each nuclear spin to the electron spin is different, because it depends on the overlap between the respective nuclear and electronic wave functions, encoded in weights A_k.

Many materials used in fabrication of quantum dots have zero nuclear spin. In natural silicon, 5% of the nuclei are magnetic due to the isotope ^{29}Si, in natural carbon only 1% due to the isotope ^{13}C. One of the most popular materials of quantum dots is gallium arsenide. The gallium isotopes ^{69}Ga and ^{71}Ga (which have together 99% abundance) and arsene ^{75}As, all have nuclear spin 3/2. Hence, the hyperfine coupling plays a significant role in GaAs quantum dots. When the electron is confined in the dimensions of the quantum dot, smaller than the spin-orbit scattering length, the hyperfine interaction becomes the dominant interaction of the electron spin with the environment. The importance of hyperfine interaction in two-electron double quantum dots was first suggested theoretically [45–47], and experimental verification of the singlet-triplet dephasing

was made by Johnson *et al.* [48] and Koppens *et al.* [49].

The interaction of 10^6 nuclear spins with the electron spin is demanding to model numerically. Instead, it is easier to define a mean field that approximates the hyperfine interaction

$$\sum_k^N A_k \mathbf{I}_k \cdot \mathbf{S} = g\mu_B \mathbf{B}_N \cdot \mathbf{S}. \tag{3.4.2}$$

This magnetic mean field is called the hyperfine field. In the absence of strong nuclear spin polarization, the hyperfine field has random values for different spatial coordinates and its average is zero. Normally, the nuclear spins are only weakly polarized in the direction of an external magnetic field. If all the nuclear spins in GaAs are completely polarized, the nuclear field can be as high as 5 T. The confined electron of the quantum dot overlaps with N surrounding nuclei. The spins of these nuclei fluctuate randomly. The root mean square of the hyperfine field is $B_{N,max}/\sqrt{N}$. The variation of the hyperfine field causes the dephasing of the initial state. It is possible to determine N from the dephasing time of the quantum dot states. In GaAs, the experiments give $N \approx 10^6$ for the number of nuclear spins overlapping with the confined electron [43].

The hyperfine field, even if it is much smaller than the external magnetic field, has a profound effect on the spin dynamics. In the case of two electrons confined in a double quantum dot, the hyperfine field has different magnitude and direction for the two dots. The singlet and triplet states are coupled if the effective magnetic fields of the two dots differ [50]. The hyperfine field thus gives rise to this coupling. The nuclear spin is much more weakly coupled to the magnetic field than the electron spin. The gyromagnetic ratio of a free electron is $\gamma_e = -g_e\mu_B/\hbar$ =-28 GHz/T. On the other hand, the gyromagnetic ratio of nuclei $\gamma = g\mu_N/\hbar$ is -24 Mhz/T for ^{69}Ga, -30 Mhz/T for ^{71}Ga, and -17 Mhz/T for ^{75}As. The magnetic coupling of GaAs nuclei is thus thousand times smaller than the magnetic coupling of the electron, and the external magnetic field does not cause a significant net polarization of nuclear spins.

3.4.3 Decoherence of spin states in quantum dots

In quantum dots, the decoherence of spin states is most often due to spin-orbit or hyperfine interactions. The hyperfine interaction is present only in materials with nonzero nuclear spin. In a two-electron double quantum dot, the singlet state S and triplet state T_0 are coupled both with spin-orbit and hyperfine interactions, but the spin-orbit coupling vanishes in the lowest order, making hyperfine interaction the dominant interaction.

The decoherence mechanisms of electron spin states in quantum dots can be divided into energy relaxation, in which the spins flip, and dephasing, where the spins lose their phase coherence, but conserve their net magnetic momentum. In general, dephasing means the decay of off-diagonal elements of the density matrix in the energy eigenbasis of the system. According to the established notation, originating from nuclear magnetic resonance (NMR) spectroscopy, the spin-relaxation time is called T_1 and spin-dephasing time is called T_2. It can be shown that $T_2 \leq 2T_1$, i.e., the dephasing is always faster than relaxation [51]. The time scale when the electron phase is randomized during the evolution without losing the phase coherence is denoted with T_2^*. The phase coherence can be restored, e.g., with a spin echo pulse [52, 53]. T_2^* is usually much smaller than T_2. For efficient quantum computation, the spin manipulation time should be both smaller than T_2^* and many orders of magnitude smaller than T_2 in order to fulfill the DiVincenzo criterion for long decoherence times.

The random fluctuations of the 10^6 nuclear spins coupled to the electron spin in the quantum dot give rise to randomness of the hyperfine mean field. The strength of the hyperfine field is usually of the order of 1 mT. These local differences in the hyperfine field cause a phase difference between the spin states of the electrons. During the measurement, the hyperfine field changes its orientation many times. The measurement result is thus an average over different nuclear spin configurations. This phase variation between measurements leads

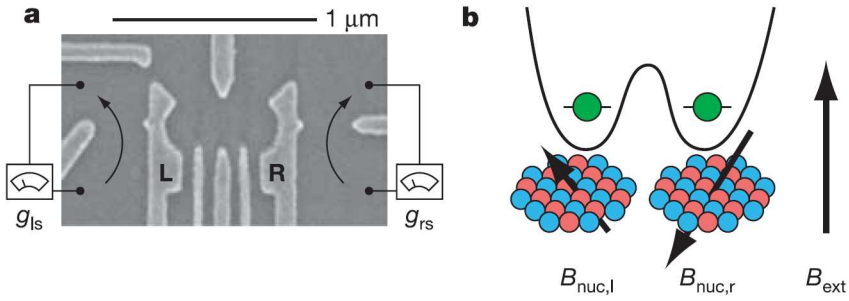

Figure 3.6: Electrostatically controlled double quantum dot. The electrons in the two dots have different nuclear spin environments leading to different nuclear mean fields (adapted from Ref. [48] by Johnson *et al.*).

to hyperfine dephasing, with time T_2^* of the order of 10 ns. The dephasing can also be due to magnetic field gradient, which could be induced by applying different magnetic fields to the different dots.

The dephasing can be controlled by applying spin echo pulses that induce the electron spins to return to the same phase [54]. The nuclear spins interact weakly with the environment, and the time scale of nuclear spin precession is often in the range of milliseconds or even seconds. Hence, if the spin echo pulses are shorter than the nuclear spin precession time, the spin phase coherence can be maintained. The spin echos have to be repeated regularly to prevent the increase of phase differences.

The precession of the nuclear spins does not have a considerable effect to the mean hyperfine field, as the different spin orientations are averaged. If the net polarization of the nuclear spins changes (dynamical nuclear polarization), it affects the hyperfine field. Also if two nuclear spins with different hyperfine couplings change simultaneously (so that the total spin is conserved) the hyperfine field changes. The nuclear spins could make a flip-flop with the electron spin, in

which one electron spin flips from down to up and one nuclear spin flops from up to down. The flip-flop process is mainly due to the hyperfine field component perpendicular to the external magnetic field. If the external magnetic field is much larger than the perpendicular hyperfine field, the separation between the electron-spin states becomes too large for the electron-nuclear flip-flops.

The nuclear spins change orientation mainly due to the dipole-dipole interaction between nuclei and the hyperfine interaction between nuclei and electrons. The time scale of nuclear dynamics due to the dipole-dipole interaction in GaAs is quite long, 100 μs [55], due to the weak interaction strength of the order of 0.01 neV [43]. The hyperfine interaction causes not only precession of the electron spin due to the coupling to nuclei, but also the nuclear spins precess about the hyperfine field due to the surrounding electrons. The hyperfine field experienced by the nuclei is called the Knight shift and the strength of this field is between 0.1 neV and 10 neV [43]. The nuclear spins evolve in this field in 10 μs time scale [46, 56, 57]. In the presence of a large (over 100 mT) magnetic field, the fluctuations of the hyperfine field parallel to the magnetic field are suppressed and the parallel field is constant over a millisecond time scale. The perpendicular field varies in a 10-100 μs time scale due to dipole-dipole and hyperfine interactions. If the electron and nuclear spin splittings differ too much, the direct flip-flop process is not likely, but virtual flip-flops can take place. Two nuclear spins can flip successively with one electron spin, so that after the process, the electron spin remains in its original orientation. It is assumed that these virtual processes are the main cause to the nuclear field fluctuations in the microsecond time scale.

In the case of two-electron double quantum dots, the hyperfine coupling causes dephasing between singlet and triplet states. The triplet states T_+ and T_- can be decoupled from the singlet state by increasing the magnetic field so that the Zeeman energy splits these states from the singlet state. The energy splitting J between S and T_0 can be controlled by changing the external detuning voltage ε

over the quantum dot. The Hamiltonian of the system in S-T_0 basis reads

$$\begin{pmatrix} 0 & g\mu_B \Delta B_{N,z} \\ g\mu_B \Delta B_{N,z} & J(\varepsilon) \end{pmatrix}.$$

We find that the off-diagonal element that gives the coupling depends on the difference of the hyperfine magnetic field component parallel to the external magnetic field. The energy difference J can be controlled with the detuning ε so that the singlet and triplet energies cross at a certain detuning value. Near the crossing point, singlet-triplet transitions are possible, but further away from the crossing the energy difference prevents transitions.

Usually, the dephasing measurements in two-electron double quantum dots are performed so that the system is first initialized in the singlet state by setting a large value of ε. In that case, both electrons are in the same dot, where only the antisymmetric singlet state is possible. Then, ε is lowered to zero so that the potentials in both dots become degenerate and one electron can move to the other dot. When the electrons are in different dots, the symmetric T_0 state is degenerate with the singlet state. The electrons are in different hyperfine fields. This difference of fields causes different spin precession rates for the electron spins, leading to dephasing between the singlet and triplet states. After free singlet-triplet evolution, the energy difference is raised back to its original value, and the state of the system is measured with charge sensing techniques. The singlet probability is obtained by taking average over a large number of measurements. By varying the length of time interval when the detuning is kept in its smallest value, one can measure the time dependence of the singlet probability. The dephasing time scale is of the order of 10 nanoseconds. Measurements of singlet-triplet dephasing are presented in Fig. 3.7.

The Hamiltonian of the two-electron system is of the same form as the one in the Landau-Zener model. In the vicinity of the crossing point, one can approxi-

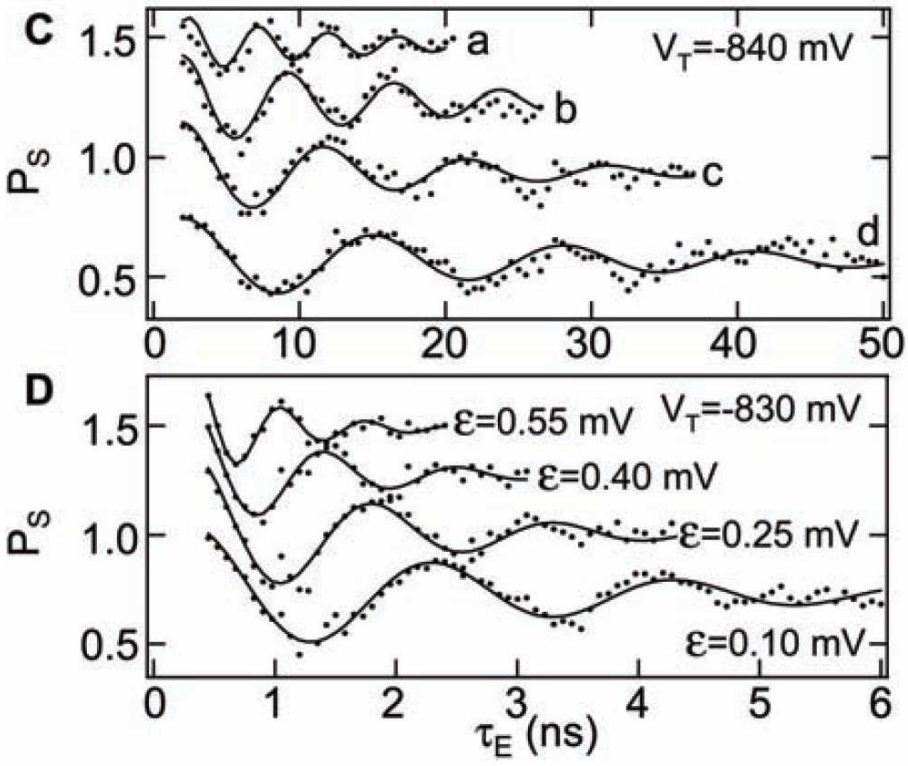

Figure 3.7: Singlet-triplet dephasing from the experiment of Petta *et al.* [13]. Horizontal axis gives the singlet-triplet dephasing time, vertical axis gives the singlet probability. The curves are offset by 0.3 for clarity. An exponentially damped cosine is fitted to the measurements.

mate that the energy difference is a linear function of detuning $J(\varepsilon) = K\varepsilon$. If the detuning is changed linearly as a function of time, one can control the occupation of singlet and triplet states by varying the changing speed of the detuning. The singlet probability, according to Landau-Zener formula, depends only on the hyperfine coupling and the time derivative of detuning.

The most popular material in quantum dots has so far been GaAs, but the effects due to nuclear spins have encouraged the studies of other materials for quantum dots with zero nuclear spin. Silicon has been studied, and especially carbon in its different allotropes, carbon nanotubes, graphene, and diamond. Carbon and silicon have also isotopes with nonzero nuclear spins, but the purification methods make it possible to get completely rid of those isotopes and hyperfine dephasing.

3.5 Electron spins as qubits

At low temperatures and in the presence of an external magnetic field, the spin states of a single electron in a quantum dot form a system that has two clearly distinct states, spin up and spin down, that are energetically well separated. In 1998, Loss and DiVincenzo proposed that electron spin could be used as a qubit [58]. Single spins are rotated with oscillating magnetic field on resonance with the electron Zeeman splitting. Two-spin rotations are made by controlling the exchange coupling between spins in neighboring dots with gate voltages. With proper exchange pulses, desired two-qubit operations can be made. The individual control of each electron spin with varying magnetic field is very challenging. One should be able to rotate one spin without affecting the direction of the other spins. If one defines the qubits as a combination of spins, one can use other control methods. The lowest-lying quantum states of the two-electron double quantum dot are singlet and triplet states. The qubits can be constructed

from these states in several ways. If one defines the orientation of a single spin as qubit, T_+ and T_- are directly two-qubit states, and the two other states are $|\uparrow\downarrow\rangle = 1/\sqrt{2}(|S\rangle + |T_0\rangle)$ and $|\uparrow\downarrow\rangle = 1/\sqrt{2}(|S\rangle - |T_0\rangle)$.

Alternatively, one can set $|S\rangle$ and $|T_0\rangle$ as qubit states. The benefit of this basis is that the states can be manipulated with electrical voltage that changes the exchange coupling. The rotations between singlet and triplet states are possible when there is a magnetic field gradient between the dots. The spin coupling with random nuclear spins induces such a gradient. Recently, a three-spin qubit of three electrons in a triple quantum dot has been experimentally studied [59]. Already in 2000, DiVincenzo *et al.* [60] proposed such a qubit. It has the advantage that an inhomogeneous magnetic field and spin rotations are not needed. Only exchange control is necessary to manipulate the qubit.

3.6 Manipulation of electron spins in quantum dots

During the past decade, the control methods of electron spins in quantum dots have attained a high level of expertise. Both electrical and optical techniques have been used for the control and readout of spin states [61, 62]. Here, we review the experiments where electrical control was used. At first, the objective of the experiments was to control and measure a single spin in a quantum dot. This was first achieved in 2001 by Fujisawa *et al.* [63] using rapid voltage pulses. They observed that the spin decay time was 10^4 times higher if the transition between states was forbidden by the spin-selection rules. The next step of spin measurements was taken in 2004 by Elzerman *et al.* [64], when they added a charge sensor to the voltage pulse scheme. This enabled the measurement of the dot charge with one-electron accuracy. The measured relaxation times for the spin states were in the millisecond regime.

The realization of two-qubit states is essential in order to make a spin qubit, as

quantum computation demands two-qubit gates. The coupling of the electron spin states is determined by the exchange energy. If the exchange energy can be properly tuned, two-qubit operations can be realized. The existence of singlet and triplet states in double quantum dots was found by Ono *et al.* [65] from the Pauli spin blockade that suppressed the current through the dot in one direction. The hyperfine coupling was soon found to mix singlet and triplet state and lift the blockade [48, 49]. In 2005, Petta *et al.* [13, 66] succeeded in controlling the exchange coupling and produced coherent two-spin oscillations.

Soon afterwards, the oscillations of a single electron spin in a double quantum dot setup were studied by Koppens *et al.* using electron spin resonance (ESR) [12, 67, 68]. Oscillating magnetic field that is perpendicular to the external static magnetic field causes coherent single-spin rotations, when the oscillating field frequency matches the energy difference of the spin states. One can also induce spin rotations by creating a position-dependent magnetic field. If the electron is perturbed so that it oscillates spatially, the electron in its rest frame is in an oscillating magnetic field, inducing electron spin rotation. The local control is easier for electric fields than for magnetic fields, which makes it easier to perform single-qubit operations. The group of Koppens managed to control the single spin rotations with oscillating electric field [69].

One can adjust the coupling of singlet and triplet states by polarizing the nuclear spins surrounding the quantum dot. When the two-spin system is driven through $S - T_+$ crossing, the flipping of one electron spin induces polarization of the nuclear spins. When the system is repeatedly driven through the singlet-triplet crossing, the net nuclear spin polarization increases. This phenomenon is called dynamic nuclear polarization, and it has been realized experimentally [70, 71] and the control of the singlet-triplet coupling with dynamic nuclear has been demonstrated [72].

The manipulation of the lowest-lying energy levels of the double quantum dot

with gate voltages enables Landau-Zener transitions between the two lowest energy levels. The gate voltage pulses can be carefully designed so that the speed of the energy level crossing can be controlled. If the system is initially in the singlet state, it is in a superposition of singlet and triplet state after the Landau-Zener transition. An experimental realization of consecutive Landau-Zener crossings and ensuing coherent singlet-triplet oscillations was recently presented by Petta *et al.* [73].

Chapter 4

Computational methods

4.1 Numerical methods for solving the Schrödinger equation

In this Thesis, the dynamics of quantum mechanical systems has been the main object of study. The dynamics has been studied with the help of different numerical computation methods. For the numerical methods, we set a discrete two-dimensional numerical grid on the quantum dot. For two electrons, we need four coordinates to indicate the positions of the electrons, making our system four-dimensional. The Schrödinger equation describing the system has to be transformed to a discrete form. This is done using finite-difference method for the derivatives appearing in the Hamiltonian. Once we have formulated the Hamiltonian, we need to diagonalize it for the calculation of eigenvalues and eigenvectors. We perform the diagonalization using the Krylov techniques.

The size of the Hamiltonian matrix becomes large when the number of grid points increases. For 20 points in one direction, the matrix size is 160 000. The calculation of so many matrix elements is quite slow. We are interested only in the lowest eigenvalues of the system. In that case, we can use Krylov subspace

methods, where we only need to know the product of the Hamiltonian with the basis function. The lowest eigenvalues are then found using the Lanczos diagonalization method. The Lanczos method can also be used for the diagonalization of the Hamiltonian in the calculation of the exponential of the Hamiltonian matrix, relevant to the calculation of the two-electron dynamics. In the following subsections, we present generally these numerical methods that were used in the calculations of the results presented in this Thesis.

4.1.1 Finite-difference method

The Schrödinger equation is a differential equation. In order to solve it numerically with discrete time steps, we can use the finite-difference method for the first and second-order derivatives that occur in the equation. In the case of external magnetic field, the momentum operator $(-i\hbar\nabla + e\mathbf{A})^2$ contains, in addition to the Laplacian ∇^2, the cross-term $\nabla \cdot \mathbf{A}$, where $\mathbf{A}$ is the vector potential of the magnetic field, $\mathbf{A} = \nabla \times \mathbf{B}$. We set a grid on the plane of the two-dimensional electron gas. For simplicity, we use below the same grid spacing h in x and y directions, although in numerics the grid spacings are chosen independently of each other. We use the four nearest neighboring points both in the x and y-direction in the evaluation of the finite differences. The second-order two-dimensional Laplacian reads in the five-point finite-difference approximation [74]

$$\begin{aligned}\nabla^2 f(x,y) &\approx [-f(x-2h,y) + 16f(x-h,y) + 16f(x+h,y) - f(x+2h,y) \\ &- f(x,y-2h) + 16f(x,y-h) + 16f(x,y+h) \\ &- f(x,y+2h) - 60f(x,y)]/(12h^2) + O(h^4), \end{aligned} \tag{4.1.1}$$

and the first-order derivative takes the form [74]

$$\begin{aligned}\nabla f(x,y) &\approx [f(x-2h,y)-8f(x-h,y)+8f(x+h,y)\\ &- f(x+2h,y)+f(x,y-2h)-8f(x,y-h)\\ &+ 8f(x,y+h)-f(x,y+2h)]/(12h)+O(h^4). \qquad (4.1.2)\end{aligned}$$

4.1.2 Exact diagonalization

In quantum mechanics, one is interested in the solution of the time-independent Schrödinger equation $\hat{H}|\psi\rangle = E|\psi\rangle$. The state vectors of the system are in the infinite-dimensional Hilbert space. A very common procedure in exact diagonalization is to divide the Hamiltonian operator into two parts $\hat{H} = \hat{H}_0 + \hat{H}_I$, where $\hat{H}_0$ is the analytically solvable part. We choose eigenstates of $\hat{H}_0$ as the orthonormal basis functions $|\phi_i\rangle$ for the construction of the elements of matrix H. Thus, we insert the expansion $|\psi\rangle = \sum_i \alpha_i|\phi_i\rangle$ into the Schrödinger equation $\hat{H}|\psi\rangle = E|\psi\rangle$ and obtain

$$(\hat{H}_0 + \hat{H}_I)\sum_i \alpha_i|\phi_i\rangle = E\sum_i \alpha_i|\phi_i\rangle, \qquad (4.1.3)$$

which can be converted to a matrix equation by multiplying $\langle\phi_j|$ to the left

$$\sum_i (H_0 + H_I)_{ji}\alpha_i = E\alpha_j, \qquad (4.1.4)$$

where the matrix elements are $H_{ji} = \langle\phi_j|H|\phi_i\rangle$, and $\alpha = (\alpha_1, \alpha_2, ...)^T$. This equation can be presented as a matrix equation $H\alpha = E\alpha$. One has to truncate the infinite basis to calculate the matrix elements. Although the term *exact diagonalization* is used, the results are exact in the limit of infinite basis. The exact diagonalization method has been widely used by quantum chemists, who call it configuration-interaction (CI) method. The name comes from the principle that

the eigenstates of the non-interacting many-body problem are called configurations and the interaction matrix elements are the configuration interaction.

In this Thesis, we do not use these kind of basis functions. Instead, we use the interacting two-electron Hamiltonian obtained from the finite difference method. The basis function are the two-electron configurations, i.e., all the possible positions of the two electrons in the numerical grid. The size of this Hamiltonian becomes quite large. For the diagonalization of the Hamiltonian, we have to use Krylov subspace methods to simplify the problem.

4.1.3 Lanczos diagonalization

The many-body basis size depends exponentially on the particle number. Although the Hamiltonian matrix is sparse, the complexity of the many-body problem grows high for large electron numbers. In many cases, we need information only on the ground state and the lowest excited states of the system. Such states can be calculated efficiently using the Krylov subspace methods [75, 76]. With these methods, it is not necessary to save all the matrix elements, but it is sufficient to evaluate the matrix-vector multiplication $H\psi$.

The Lanczos diagonalization method is an iterative algorithm, developed by a Hungarian mathematician Cornelius Lanczos, for finding eigenvalues and eigenvectors of a square matrix [76–78]. It is especially useful for large sparse matrices. Such matrices often arise when Schrödinger equation is discretized with finite-difference method. The eigenvalues and eigenstates with lowest energies are easy to find with Lanczos method. The aim of the iterative method is, given a Hermitian matrix A, to find a Hermitian tridiagonal and symmetric matrix $T_m = V_m^* A V_m$ during m iteration rounds. The eigenvalues of T_m are then easy to calculate. The main advantage of the Lanczos iteration is that even if the number of iterations is much smaller than the dimension of A, the eigenvalues of T_m are good approximations of the eigenvalues of A. The smallest eigenvalues

are approximated better than the higher ones, because sometimes the eigenvectors corresponding to higher eigenvalues are not orthogonal due to numerical inaccuracies. Another benefit of the Lanczos iteration is that for iteration round $j+1$, we only have to form product of matrix A with vector v_j, we do not need to calculate the matrix elements.

4.1.4 Matrix exponential

When we study the dynamics of a quantum-mechanical system, we need to solve the time-dependent Schrödinger equation $i\hbar\frac{\partial}{\partial t}\psi = H\psi$ with the initial condition $\psi(t=0) = \psi_0$. When the Hamiltonian is time-independent, the solution is $\psi(t) = \exp(-iHt/\hbar)\psi(0)$. If the Hamiltonian is time-dependent, we may still use the same approach in the discretized version $\psi(t+\Delta t) = \exp(-iH(t)\Delta t/\hbar)\psi(t)$. The solution contains an exponential of the Hamiltonian matrix. The matrix exponential is defined as

$$\exp(A) = \sum_{k=0}^{\infty} \frac{1}{k!} A^k. \tag{4.1.5}$$

The construction of the exponential as a sum of multiplications of a matrix causes that the exponential of a sparse matrix is a dense matrix. It would thus be desirable to avoid computing the exponential from the definition.

Several methods are used to compute the matrix exponential [79]. For our purposes, the Krylov subspace methods for the exponential are the most suitable ones. We calculate the exponential of the Hamiltonian matrix by using the unitary transformation of the Hamiltonian into a diagonal form $H = V\Lambda V^\dagger$, where Λ is a diagonal matrix containing the eigenvalues, and V is a unitary matrix containing the eigenvectors of the Hamiltonian. Then, we may express the exponential of the Hamiltonian as

$$\exp(-iHt/\hbar) = \exp(-iV\Lambda V^\dagger t/\hbar) = V\exp(-i\Lambda t/\hbar)V^\dagger. \tag{4.1.6}$$

For interacting electrons, the size of the Hamiltonian matrix becomes very large. For example, for two electrons we need four-dimensional space, and with discretization of 20 points in one direction the size of the matrix is 160 000 elements. Although the Hamiltonian matrix is large, it is also sparse. For the evaluation of the exponential, we need to calculate the eigenvectors and eigenvalues. Now, the Lanczos method proves very useful. When we use Lanczos diagonalization for calculation of the eigenvalues and eigenvectors, we do not need to store the elements of the Hamiltonian matrix, because we only have to know the product of the Hamiltonian with the wave function, which turns out to be easy to calculate. The dynamics of the system is dominated by the lowest eigenstates of the system. It turns out that if the dimension of the Krylov subspace is at least 50, the dynamics is well estimated. For accurate calculation of the dynamics, the time step δt has to be short, of the order of 100 fs. To reach the time scales of the decoherence phenomena in quantum dots, occurring in nanosecond and microsecond regime, we need between 10^4 and 10^7 time steps in the calculation. The reduction of the large Hamiltonian to a small matrix is necessary in order to achieve reasonably rapid computation of the dynamics.

4.2 Evaluation of the effect of hyperfine interaction

The fluctuation of the hyperfine field couples the singlet and triplet states. For different hyperfine fields, the system evolves unitarily. The singlet-triplet decoherence is due to phase averaging that is evaluated by averaging the unitary evolutions of the system. The two-dimensional grid used in the calculation of the dynamics of the quantum dot is quite sparse due to the complexity of the calculation. The time propagation of the system would become too slow if there are too many grid points. Therefore, only 20-30 data points are used in one direction. In each point of the grid, the hyperfine field value represents a mean field of the hyperfine spins that are closest to this grid point.

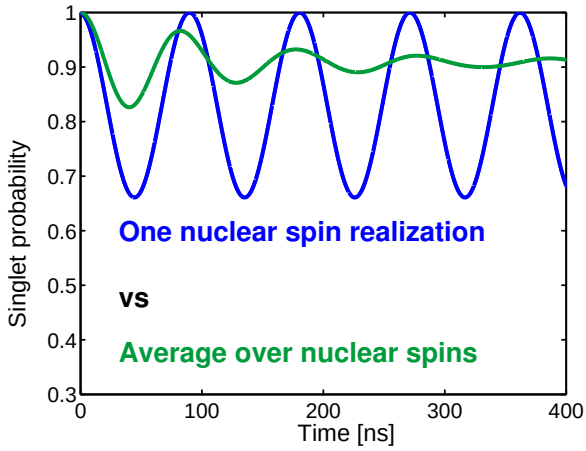

Figure 4.1: Phase averaging of the singlet oscillations.

The orientations of the hyperfine spins can be considered to be normally distributed. In practice, the singlet-triplet decoherence is the same if uniform distribution is used instead of normal distribution. In each grid point, the hyperfine mean field is set to a random value. Because the grid is sparse, the hyperfine fields of neighboring grid points are not correlated and can be randomly set independent of each other. The width of the hyperfine field distribution in the calculation depends not only on the physical parameters, but also from the details of the numerical calculation. If the grid spacing is increased, the hyperfine mean field of each point is an average over a larger number of hyperfine spins and the strength of the hyperfine field diminishes. Thus, the width of the hyperfine field distribution can not be directly deduced from the measurements, but it is fitted to the measurement data so that the singlet-triplet probability has the same asymptotic value in the experiment and numerical simulation.

The unitary evolution of the system is calculated using different realizations of the hyperfine field. The amplitudes and periods of the singlet oscillations for the realizations vary. As a result, the average over the realizations is a decaying

oscillation. In Fig. 4.1, the effect of averaging is illustrated. It should be noted that the fluctuations of the nuclear field have clearly longer period (over 1 μs) than the singlet-triplet decoherence time (of the order of 10 ns). Even for spin dynamics calculations for times of the order of 100 μs, one can assume that the nuclear field is constant. The value of the hyperfine field has an effect on the spin dynamics only near the singlet-triplet transition point. During the change of the external system parameters, the transitions between the spin states take place in a microsecond time scale.

Chapter 5

Discussion

This Thesis discusses physical phenomena in semiconductor two-electron quantum dots and the theory describing these phenomena. The main topic of this Thesis has been the study of two-electron dynamics and decoherence in quantum dots. The main cause of decoherence of the spin states in GaAs quantum dots is the hyperfine interaction between electron spin and spins of the nuclei surrounding the electron. We have developed numerical methods in order to calculate the two-electron dynamics and to investigate the effect of the hyperfine interaction. We approximate the hyperfine interaction with a random magnetic field, and calculate the two-electron dynamics exactly using diagonalization of the finite difference Hamiltonian. This approach for the dynamics has been used in all publications included in this Thesis.

The lowest energy states of two-electron quantum dots are the singlet and triplet states. Recent experiments have investigated the decoherence of these states, which has motivated our choice of research topic and enabled the comparison of our numerical results with experimental data. Our studies also discussed the effects of the polarization of the nuclear spins on the decoherence. The transitions between the singlet and triplet states have been experimentally realized by tuning the external gate voltage over the quantum dot. We proposed a novel scheme

to induce these transitions with a time-dependent external magnetic field both in a quantum dot and a quantum ring. In addition to the numerical methods, we have also calculated analytically the singlet-triplet transition probabilities. The development of surface-acoustic wave (SAW) quantum dots encouraged us to study the charge dynamics of a two-electron quantum dot under changing SAW potential.

There have been only a few measurements on the decoherence in two-electron quantum dots. The group of Jason Petta in Harvard has produced some of the most important publications of this field during recent years. In 2006, they measured the singlet-triplet decoherence in a double quantum dot for different values of exchange interaction [66]. The experimental data showed a large variance of the asymptotic singlet probability.

In Publication **I**, we modeled the experiment numerically and explained that the variance of the singlet probability is due to the limited number of measurement used in the averaging of the probabilities. The dynamics of the probabilities was in good agreement between measurements and our calculations. In this Publication, we assumed that the nuclear spins are unpolarized. The effect of polarization was discussed in Publication **II**, using analytical and numerical methods to calculate the singlet probability and its variance. We used a simplified effective Hamiltonian in the analysis. Our results indicated, that a small polarization does not considerably affect the dynamics, and suggest that a large hyperfine spin polarization could be observed using experimental methods.

In two-level quantum systems, the transitions between the two states may be adiabatic, nonadiabatic, or a combination of both, leading to a superposition state. The type of the transition depends on the changing speed of the external parameters and of the coupling strength between the two states, according to the Landau-Zener formula. We studied the possibility to induce transitions between the singlet and triplet states using external time-dependent magnetic field

in two-electron double quantum dots (Publication **III**) and in quantum rings (Publication **IV**). By adjusting the speed of the magnetic field change, the occupations of the spin states can be controlled. We calculated the strength of the magnetic field and the time scale of the magnetic field manipulation that is needed to efficiently control the spin states. The distribution of the asymptotic singlet probability was also studied. In the future, the proposed method could be used to manipulate the singlet and triplet states, although the rapid control of the magnetic field is quite demanding to realize.

Consecutive singlet-triplet transitions with different external voltage values were recently measured by Petta *et al.* [73]. As a result of these crossings, the singlet probabilities form an interference pattern, when the measured probabilities with different voltages are shown in a single figure. The observed decay of the singlet oscillations is in accordance with our numerical results. We explained the interference observed by Petta *et al.* in Publication **VI**, and suggested that the interference of the singlet state with two different triplet states is possible and could be observed in future experiments, if the measurement visibility is high.

Recently, the coherent time evolution of a single-electron wave function was measured in a single-electron SAW quantum dot by Kataoka *et al.* [33]. This encouraged us to study the dynamics of a two-electron wave function in SAW quantum dot in Publication **V**. Two electrons are initially in a single dot. The confinement potential is suddenly changed so that the a double dot is formed. We showed that by choosing a suitable external magnetic field, or by applying an oscillating external voltage, one can induce both one-electron and two-electron oscillations between the dots. We studied the amplitude and periodicity of these charge oscillations and the effect of the periodic external potential. Our results might help experimentalists two develop SAW dots further.

In summary, the two-electron spin and charge states in two-dimensional quantum dots exhibit rich dynamics. The dynamics of the quantum states of the elec-

trons can be controlled with the external parameters such as magnetic field and external voltage. The effect of the hyperfine interaction on the spin states can be regarded both detrimental, as the decoherence causes difficulties for the qubit control, and beneficial, because the singlet-triplet coupling can be harnessed to control the occupation of the dot states. The results of this Thesis might give future experimentalists guidance how the environmental coupling can be used as an advantage in the rising field of quantum computation.

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Technological advances have enabled manufacturing of nanometer-sized semiconductor quantum dots, where a small number of electrons is confined. The charge of the quantum dot can be controlled at one-electron level, and the spin of the confined electron can be used as a quantum bit, an information unit of a quantum computer. Realization of a working quantum computer requires study of the dynamics and decoherence of the electron states of the quantum dot, which are the topics of this Thesis. The research in this work is carried out using numerical and theoretical methods, comparing results with latest experimental studies. Hyperfine interaction of the confined spins with nuclear spins of the surrounding material is a major cause of decoherence, and is thus investigated in detail. New methods for controlling the quantum dot states are also proposed.

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